

Hydrogen cyanide
74-90-8 | DTXSID9024148

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 9.91 days

Global applicability domain: Outside

Local applicability domain index: 2.16e-01

Confidence level: 8.64e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Pentane</div> <div>Measured: 40.7</div> <div>Predicted: 6.52</div>	<div>Image not found</div> <div>Tridecane</div> <div>Measured: 305</div> <div>Predicted: 13.5</div>	<div>Image not found</div> <div>Dodecane</div> <div>Measured: 201</div> <div>Predicted: 10.6</div>
<div>Image not found</div> <div>Tetradecane</div> <div>Measured: 1370</div> <div>Predicted: 18.3</div>	<div>Image not found</div> <div>Undecane</div> <div>Measured: 88.3</div> <div>Predicted: 8.56</div>	